Optimized mean-field theory for the three-dimensional XY spin model

M. E. Gouvêa and A. S. T. Pires
Departamento de Física, Instituto de Ciencias Exatas, Universidade Federal de Minas Gerais Belo Horizonte, CEP 30161, Minas Gerais, Brazil

(Received 30 May 1996)

Many physical systems of interest can be mapped into the planar rotator and XY magnetic models. We show here that the very simple approach known as the Onsager reaction field when applied to different arrangements (sc, bcc, and fcc) for the three-dimensional planar rotator model predicts values for the transition temperature which compare quantitatively well to values obtained by more sophisticated theories. For the XY model, we propose a renormalization of the exchange parameter so that the fluctuations of the out-of-plane spin component are taken into account: the results are compared to high-temperature series expansion data. [S0163-1829(96)08546-3]

Many important systems can be mapped into the plane-rotator and XY magnetic models. One example of this is the Josephson-junction arrays. It is well known that Josephson junctions offer excellent opportunity to study fundamental concepts of condensed matter because of the large variety of phenomena — ranging from nonlinear effects such as chaos and soliton dynamics to superconductivity (Ref. 3) — embodied by these systems. Josephson-junction arrays are superconducting islands coupled to form one-, two-, or three-dimensional lattices. In general, the superconducting grains are weakly coupled and at low temperatures the order parameter has a fixed modulus which is independent of any supercurrent flow. In this limit, it is the phase of the order parameter only which remains a degree of freedom for each grain and the corresponding expression for the free energy indicates that the system belongs to the class of XY classical models with a temperature-dependent coupling energy.[1,2]

It is relevant, then, to have methods for calculating some properties of XY models, as the transition temperature T_c, spin correlation lengths, etc. Usually, most of the methods available as, for example, spin-wave theories,[4–6] spin Green-function approaches[7] and Monte Carlo calculations are quite sophisticated and require lengthy calculations. It has been discussed recently,[8,9] that the Onsager reaction field (ORF) formalism, despite its great simplicity, captures many of the essential features of the model studied and provides good quantitative agreement to data obtained via more sophisticated techniques.

In this report we apply the ORF procedure to the three-dimensional (3D) plane rotator and XY models for sc, fcc, and bcc lattices. We will show that the values estimated for T_c are in close agreement to the ones obtained by high-temperature series expansion (HTSE). We remark that in the XY model the spins are not restricted to the XY plane, as they are in the plane rotator model. In fact, the dynamical properties of the XY model depend on the out-of-plane fluctuations. We propose a self-consistent way to take into account these fluctuations in the ORF calculation done for the planar rotator model. The comparison to HTSE data is, again, very good.

The ORF formalism represents an improvement over the usual mean-field approximation because it includes short-range effects. The basic idea is that the spins surrounding any given spin will be correlated to the motion of that spin and, therefore, will not contribute to the mean field seen by that spin: this is incorporated into the theory by subtracting the reaction field of the mean field. The ORF was first used in magnetism by Brout and Thomas[10] and has since been applied successfully to spin glasses[11,12] to itinerant-electron systems[13] and to the Heisenberg model.[6,8,9]

The Hamiltonian for the plane-rotator and for the XY model is given by the same expression

$$\mathcal{H}=-2J\sum_{\langle i,j\rangle}(S_i^xS_j^x+S_i^yS_j^y) \tag{1}$$

with the remarkable difference between the two models being that in the XY model $S_z\neq 0$. In the above equation, i specifies a site in the lattice, J is the exchange constant, and the summation is performed over nearest neighbors only. The Fourier transform of Hamiltonian (1) is given by

$$\mathcal{H}_{\vec q}=-\sum_{\vec q} J(\vec q)(S^x_{\vec q}S^x_{-\vec q}+S^y_{\vec q}S^y_{\vec q}), \tag{2}$$

where $J(\vec q)=J\Sigma_{\vec\delta}\exp(i\vec q\cdot\vec\delta)$ with $\vec\delta$ being a vector connecting each site to its nearest neighbors. The expressions for $J(\vec q)$ for the three lattices we will consider here are given by

$$J(\vec q)=2J(\cos q_x+\cos q_y+\cos q_z),\quad \text{for sc},$$

$$J(\vec q)=8J(\cos q_x\cos q_y\cos q_z),\quad \text{for bcc},$$

and (3)

$$J(\vec q)=4J(\cos q_x\cos q_y+\cos q_x\cos q_z+\cos q_y\cos q_z),\quad \text{for fcc}.$$

In the mean-field (MF) approximation, the susceptibility is simply given by

$$\chi=\frac{\chi_0}{1-\chi_0 J(\vec q)}, \tag{4}$$

where $\chi_0=S^2/2T$. The MF critical temperature, T_c^{MF}, corresponds to the temperature which satisfies $J(\vec 0)=\chi^{-1}$. The first column of Table I gives T_c^{MF} for the plane-rotator: as can

0163-1829/96/54(21)/14907(3)/$10.00

TABLE I. Critical temperatures for the plane-rotator and XY 3D models for sc, bcc, and fcc lattices. The first column gives the mean field estimative; third and fourth columns correspond, respectively, to the ORF and renormalized-ORF approaches. The data given in the second and fifth columns correspond to HTSE results for the plane-rotator and XY models, respectively. The sixth column corresponds to $J(\vec{0})$ as given by Eq. (3).

	$\mathrm{MF_{RP}}$	Rotor*	ORF	$\mathrm{ORF}_{\tilde{J}}$	XY*	$J(\vec{0})$
sc	3	2.203	1.98	1.49	1.552	6.0
bcc	4	3.121	2.87	2.11	2.175	8.0
fcc	6	4.820	4.46	3.25	3.342	12.0

be expected in a MF context, the critical temperatures are always overestimated. The relative difference between the MF result and the values obtained via HTSE (second column) decreases with the increasing of the coordination number and varies from $\approx 24\%$ for fcc lattices to $\approx 36\%$ for sc.

In order to incorporate short-range order effects into the mean field approach we must subtract from the molecular field $J(\vec{q})$ acting on a given spin the part due to the polarization by that spin, of its neighbors: this part corresponds to the ORF and since it follows the motion of the spin in question, it cannot be included in the effective orienting field. Proceeding in this way, the expression for the static susceptibility becomes

$$\chi(\vec{q})=\frac{\chi_0}{1-\chi_0[J(\vec{q})-\lambda(T)]}, \tag{5}$$

where $\lambda(T)$ is defined as

$$\lambda(T)=\sum_j \lambda_{ij}J_{ij}, \quad \text{with} \quad \lambda_{ij}=\langle \vec{S}_i\cdot\vec{S}_j\rangle \tag{6}$$

and corresponds to the Onsager correction term. This term must be determined self-consistently by requiring the susceptibility (5) to satisfy the sum rule

$$\frac{1}{N}\sum_{\vec{q}} \chi(\vec{q})=\chi_0. \tag{7}$$

Inserting Eq. (5) into Eq. (7) we obtain

$$\frac{1}{(2\pi)^3}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{d\vec{q}}{2T-\lambda-J(\vec{q})}=\frac{1}{2T}, \tag{8}$$

which is the self-consistent equation we must solve in order to determine $\lambda(T)$ for the plane-rotator.

The critical temperature T_c corresponds to the highest temperature at which $\chi(\vec{q})$ diverges, that is, in the ORF formalism, at T_c, we must have $J(\vec{0})=\chi^{-1}+\lambda(T_c)$. Using this relation in Eq. (7), we obtain the expression for T_c

$$\frac{J(\vec{0})}{2T_c}=\frac{1}{\pi^3}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi}\frac{d\vec{q}}{1-J(\vec{q})/J(\vec{0})}. \tag{9}$$

The integral on the right-hand side can be calculated numerically (see, e.g., Ref. 14) and its value is 1.5164. Using expressions (3) for $J(\vec{q})$ for the three lattices, we obtain the third column of Table I: the comparison to the HTSE data is now within 7.5% for fcc to 11% for sc lattices, much better than the comparison done with MF results. We see then that the simply ORF procedure is able to make good predictions for the transition temperature for models like the plane rotator. In the ORF treatment, we can also estimate the spin correlation length, spin correlation functions and other properties in a very straightforward way:[8,9] we will not do it here because it is beyond the scope of this work.

The out-of-plane fluctuations of the XY model cannot be taken into account in either of the approximations, MF and ORF, we mentioned here. It means that, using these procedures, we would get identical estimates for the plane-rotator and for the XY model. However, it is known that the transition temperature for the XY model for a given lattice is lower than the corresponding T_c for the plane rotator. In the following we suggest a way to include the effects of this fluctuation by a proper renormalization of the exchange coupling. In order to do this, we use the following parametrization for the spin vector

$$\vec{S}_i=S_i\left[\sqrt{1-\frac{(S_i^z)^2}{S^2}}\cos\phi_i,\ \sqrt{1-\frac{(S_i^z)^2}{S^2}}\sin\phi_i, S_i^z\right]. \tag{10}$$

Inserting this parametrization in Hamiltonian (2) we obtain

$$\mathcal{H}=-J\sum_{i,j}\sqrt{1-\frac{(S_i^z)^2}{S^2}}\sqrt{1-\frac{(S_j^z)^2}{S^2}}\cos(\phi_i-\phi_j). \tag{11}$$

For temperatures such that $(S_i^z)^2/S^2\ll 1$ we can substitute $(S_i^z)^2$ for its average value, $\langle S_i^z\rangle^2$, obtaining the following approximate expression for the previous Hamiltonian:

$$\mathcal{H}\approx-\sum_{i,j} J\left(1-\frac{\langle (S_i^z)^2\rangle}{S^2}\right)\cos(\phi_i-\phi_j). \tag{12}$$

This last expression suggests the definition of an exchange constant renormalized by out-of-plane fluctuations as

$$\tilde{J}=J\left(1-\frac{\langle (S_i^z)^2\rangle}{S^2}\right). \tag{13}$$

Equipartition gives $\langle (S_i^z)^2/S^2\rangle=T/J(\vec{0})$, which leads to

$$\tilde{J}=J[1-T/J(\vec{0})]. \tag{14}$$

Notice, however, that Eq. (14) resulted from the approximations done in obtaining Hamiltonian (12) from (11), and not from the ORF procedure. In order to assure that the low-temperature approximation used above is valid, we must restrict the temperature range to $T/J(\vec{0})\ll 1$. Using the renormalized exchange constant given by Eq. (14) into Eq. (9) we obtain, for the transition temperature, the fourth column shown in Table I: the agreement to the HTSE results for the XY model (which corresponds to the fifth column of Table I) is remarkably good. The sixth column of the table gives $J(\vec{0})$: we can verify that, in all the three cases considered here, we have $T_c \ll J(\vec{0})$, as required by the low-temperature approximation used justifying, in this way, the calculations for T_c performed here.

We conclude saying that the procedures we discussed here, the ORF for planar rotator models and its renormalized version for XY models, give good estimates for the transition temperature. Other properties of these models, as the spin correlation functions and specific heat, for example, can also be calculated and compared to experimental or Monte Carlo simulations when they become available.

This work was partially supported by CNPq-Brazil (Conselho Nacional de Pesquisas).

[1] S. Teitel and C. Jayaprakash, J. Phys. Lett. (Paris) **46**, L33 (1985).
[2] L. Jacobs, J.V. Jose, M.A. Novotny, and A.M. Goldman, Phys. Rev. B **38**, 4562 (1988).
[3] *Josephson Effects—Achievements and Trends*, edited by A. Barone (World Scientific, Singapore, 1986).
[4] M. Takahashi, Phys. Rev. Lett. **58**, 168 (1987); Phys. Rev. B **40**, 2494.
[5] F. Suzuki and C. Ishii, J. Phys. Soc. Jpn. **62**, 3686 (1993).
[6] C.M. Soukolis, S. Datta, and Y.H. Lee, Phys. Rev. B **44**, 446 (1991).
[7] D.A. Yablonskiy, Phys. Rev. B **44**, 4467 (1991).
[8] M.P. Eastwood and D.E. Logan, Phys. Rev. B **52**, 9455 (1995).
[9] D.E. Logan, Y.H. Szczech, and M.A. Tusch, Europhys. Lett. **30**, 307 (1995).
[10] R. Brout and H. Thomas, Physics (Long Island City, NY) **3**, 317 (1967).
[11] M. Cyrot, Phys. Rev. Lett. **43**, 173 (1979).
[12] P. Nozières, J. Phys. (Paris) **43**, L-543 (1982).
[13] Y.H. Szczech, M.A. Tusch, and D.E. Logan, Phys. Rev. Lett. **74**, 2804 (1995).
[14] E.N. Economou, *Green's Functions in Quantum Physics* (Springer, Berlin, 1983).